

Expansions of the interatomic potential under various boundary conditions and the transition to the thermodynamic limit

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We analyze the possible expansions of the interatomic potential $U(|\mathbf{r}_1 - \mathbf{r}_2|)$ in a Fourier series for a cyclic system and a system with boundaries. We study also the transition from exact expansions for a finite system to the expansion that is usually used in the thermodynamic limit. The analysis indicates that such transition distorts the potential of a system with boundaries, by making it cyclic.

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I. INTRODUCTION

The theoretical studies of many-particle problems use frequently the expansion of the interatomic potential $U(|\mathbf{r}_1 - \mathbf{r}_2|)$ in a Fourier series. In this case, the real finite system is replaced by an infinite one: the periodic boundary conditions are used, and the sizes of a system and the number of particles in the formulas tend to infinity at the constant ratio N/V . This procedure is called the transition to the thermodynamic (T-) limit, and it gives the below-presented expansion (1)-(3). Expansion (1)-(3) is used in the whole literature on condensed media and in statistical physics as the standard trick, without explanation. We failed to find in the physical literature the justification of that the potential of a finite system with boundaries can be expanded as the potential of an infinite system. In one of the sparse books [1], where the T-transition is explained, we can read in Sect. 7: "In our entire consideration, ... the limiting transition $N \rightarrow \infty$ is performed purely formally. We do not consider the complicated mathematical problem concerning the formulation of those conditions that should be imposed on the initial data (e.g., on the form of a potential function $\Phi(r)$) in order to ensure the performing of a strict mathematical substantiation of the legitimacy of such limiting transition." In [2], the transition $N, V \rightarrow \infty$, $N/V = \text{const}$ is substantiated by means of the consideration of a statistical sum, but no proof of the coincidence of the limits for a cyclic system and a system with boundaries was given. Therefore, the validity of the transition to the T-limit for a system with boundaries is, in fact, only a likely assumption. In this case, it is assumed that either expansion (1)-(3) is exact or the inaccuracy is insignificant and cannot lead to errors at the description of a real physical system with boundaries. For the classical systems, the use of (1)-(3) does not lead to errors and, therefore, is apparently true. However, the application of (1)-(3) to such quantum liquid as He II causes the loss of a new dispersion law [3]; this law can be obtained with the use of a more exact expansion that takes explic-

itly the boundaries into account. The recent result [3] means that, for some systems, the T-limit is the mistake in the meaning that T-limits differ for a closed system and a system with boundaries. It is worth to understand whether such result is possible and, if so, why. Since the first key step in the analysis [3] is the choice of the expansion of a potential, it is necessary, first of all, to analyze the possible expansions of the potential $U(|\mathbf{r}_1 - \mathbf{r}_2|)$ in a Fourier series under various boundary conditions and to clarify the degree of accuracy of expansion (1)-(3). This theme is considered in the present work. We will show that expansion (1)-(3) is not quite exact for the systems with boundaries and will consider exact expansions.

II. ANALYSIS OF THE EXPANSIONS OF A POTENTIAL

The standard expansion (we call it T-expansion) of an interatomic potential in the T-limit reads

$$U(|\mathbf{r}_1 - \mathbf{r}_2|) = \frac{1}{V} \sum_{\mathbf{k}}^{(2\pi)} \nu(\mathbf{k}) e^{i\mathbf{k}(\mathbf{r}_1 - \mathbf{r}_2)}, \quad (1)$$

$$\nu(\mathbf{k}) = \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy \int_{-\infty}^{\infty} dz U(r) e^{-i\mathbf{k}\mathbf{r}} \equiv \nu(k). \quad (2)$$

The symbol (2π) above sum (1) indicates that \mathbf{k} runs the values

$$\mathbf{k} = 2\pi \left(\frac{j_x}{L_x}, \frac{j_y}{L_y}, \frac{j_z}{L_z} \right), \quad (3)$$

where j_x, j_y, j_z are integers, L_x, L_y, L_z are the sizes of the system, and $V = L_x L_y L_z$. In (1)-(3), the T-limit is assumed: $L_x, L_y, L_z \rightarrow \infty$.

We can try to obtain T-expansion (1)-(3) from the integral Fourier transformations [4] (for simplicity, we consider the one-dimensional (1D) case, $L_x = L$):

$$f(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \Omega(\omega) e^{i\omega t} d\omega, \quad (4)$$

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$$\Omega(\omega) = \int_{-\infty}^{\infty} dt f(t) e^{-i\omega t}. \quad (5)$$

Let us rename: $\omega = k/k_0$, $\Omega(k/k_0) = \nu(k)$, $t = x/L$, $f(x/L) = LU(x)$ (in (4) $x \leftrightarrow x_1 - x_2$), where $k_0 = 1/L$, $L \rightarrow \infty$. We also replace $\frac{L}{2\pi} \int_{-\infty}^{\infty} dk \rightarrow \sum_{k_j=2\pi j/L}$. Then

relations (4) and (5) yield (1)-(3). In this case, it is necessary to additionally substantiate the transition from the infinite system to a finite one. Below, we will give a more strict deduction of the T-expansion that is based on the consideration of a finite system.

Consider a system of N particles in a bounded volume $x \in [0, L_x]$, $y \in [0, L_y]$, $z \in [0, L_z]$, $L_x \cdot L_y \cdot L_z = V$. The function $F(\mathbf{r}_1, \mathbf{r}_2) = U(|\mathbf{r}_1 - \mathbf{r}_2|)$ can be expanded in a Fourier series in three ways: i) by considering the vector $\mathbf{r}_1 - \mathbf{r}_2$ to be the argument (the modulus is a part of the function); it is the zero-expansion; ii) by considering the vector $(|x_1 - x_2|, |y_1 - y_2|, |z_1 - z_2|)$ to be the argument; it is the modulus-expansion; and iii) by considering \mathbf{r}_1 and \mathbf{r}_2 to be the arguments (in this case, the function includes a potential, a modulus and the difference of \mathbf{r}_1 and \mathbf{r}_2). One can also invent the infinite number of nonphysical expansions. They are proper, but it is difficult to apply them to physical models. For example, we may set $x_1 - x_2 = x_1 + x_2 - 2x_2$ in the 1D case and consider $x_1 + x_2$ and $2x_2$ to be independent arguments; other combinations can be written as well. We omit these expansions.

For three above-presented expansions, we have $x_1 - x_2 \in [-L_x, L_x]$, $y_1 - y_2 \in [-L_y, L_y]$, $z_1 - z_2 \in [-L_z, L_z]$ and $|x_1 - x_2| \in [0, L_x]$, $|y_1 - y_2| \in [0, L_y]$, $|z_1 - z_2| \in [0, L_z]$. By the Fourier-analysis rules [4], we obtain i) Zero-expansion:

$$U(|\mathbf{r}_1 - \mathbf{r}_2|) = \frac{1}{2fV} \sum_{\mathbf{k}}^{(\pi)} \nu_z(\mathbf{k}) e^{i\mathbf{k}(\mathbf{r}_1 - \mathbf{r}_2)}, \quad (6)$$

$$\nu_z(\mathbf{k}) = \int_{-L_x}^{L_x} dx \int_{-L_y}^{L_y} dy \int_{-L_z}^{L_z} dz U(r) e^{-i\mathbf{k}\mathbf{r}} \equiv \nu_z(k), \quad (7)$$

where f is the dimension of the system, and (π) above the sum indicates that \mathbf{k} runs the values

$$\mathbf{k} = \pi \left(\frac{j_x}{L_x}, \frac{j_y}{L_y}, \frac{j_z}{L_z} \right). \quad (8)$$

ii) Modulus-expansion:

$$U(|\mathbf{r}_1 - \mathbf{r}_2|) = \sum_{\mathbf{k}}^{(2\pi)} \frac{\nu_m}{V}(\mathbf{k}) e^{ik_x|x_1-x_2|+ik_y|y_1-y_2|+ik_z|z_1-z_2|}, \quad (9)$$

$$\nu_m(\mathbf{k}) = \int_0^{L_x} dx \int_0^{L_y} dy \int_0^{L_z} dz U(r) e^{-i\mathbf{k}\mathbf{r}}. \quad (10)$$

Expansion (iii) will be considered in what follows. By two one-dimensional examples, we will examine the degree of accuracy of the above-presented expansions.

Example (A) involves the expansion of a linear potential

$$U(|x_1 - x_2|) = U_0|x_1 - x_2|/L \quad (11)$$

in the domain $x_1, x_2 \in [0, L]$. In this case, the zero-series (6), (7) takes the form

$$U(|x_1 - x_2|) = \frac{U_0}{2} - \frac{4U_0}{\pi^2} \sum_{j=0,1,2,\dots} \frac{\cos[\pi(2j+1)(x_1 - x_2)/L]}{(2j+1)^2} \quad (12)$$

and reproduces (11) exactly, in the required domain. The modulus-series (9), (10) can be written as

$$U(|x_1 - x_2|) = \frac{U_0}{2} - \frac{U_0}{\pi} \sum_{j=1,2,\dots} \frac{\sin[2\pi j|x_1 - x_2|/L]}{j}. \quad (13)$$

It reproduces (11) exactly as well. For the T-expansion, we have $\nu(k \neq 0) = 0$, and the series is reduced to

$$U(|x_1 - x_2|) = \nu(0)/L = U_0. \quad (14)$$

In other words, the T-expansion distorts the initial potential. This occurs due to the addition of the “image,” namely the potential $U(L - |x_1 - x_2|)$ (see below).

Let us consider example (B) with the potential of “semitransparent balls”

$$U(|x_1 - x_2|) = \begin{cases} U_0 > 0, & 0 \leq |x_1 - x_2| \leq a, \\ 0, & a < |x_1 - x_2| \leq L. \end{cases} \quad (15)$$

In this case, the zero-series reads

$$U(|x_1 - x_2|) = \frac{aU_0}{L} + \frac{2U_0}{\pi} \sum_{j=1,2,3,\dots} \frac{\sin(\pi ja/L)}{j} \cos[\pi j(x_1 - x_2)/L] \quad (16)$$

and reproduces function (15) in the domain $x_1, x_2 \in [0, L]$ exactly. The modulus-series takes the form

$$U(|x_1 - x_2|) = \frac{aU_0}{L} + \frac{U_0}{\pi} \sum_{j=1,2,3,\dots} \frac{1}{j} \{ \sin(2\pi ja/L) \cos[2\pi j(x_1 - x_2)/L] + (1 - \cos(2\pi ja/L)) \sin[2\pi j|x_1 - x_2|/L] \} \quad (17)$$

and also reproduces potential (15) exactly. The T-expansion (15) is

$$U(|x_1 - x_2|) = \frac{2aU_0}{L} + \frac{2U_0}{\pi} \sum_{j=1,2,3,\dots} \frac{\sin(2\pi ja/L)}{j} \cos[2\pi j(x_1 - x_2)/L] \quad (18)$$

and yields the function

$$U^T(x) = \begin{cases} U_0, & 0 \leq |x| \leq a, \\ 0, & a < |x| \leq L-a, \\ U_0, & L-a < |x| \leq L, \end{cases} \quad (19)$$

which contains, in addition to the initial potential, its “image”: the same potential at the end of the interval, i.e. at $]L-a < x \leq L]$. We note that, at the points of discontinuity of the function, the expansion given the arithmetic mean of the values of the function on the left and on the right from the discontinuity, but we omit this item for simplicity. We summed all series numerically. Series (12) and (13) are summed analytically at the points $x_1 - x_2 = 0; L/4; L/2; 3L/4; L$.

The **principal point** consists in the following. If we would expand the function $f(x)$, which depends on the single argument and is given on the interval $x \in [0, L]$, in a Fourier series, then the Fourier series would yield the function $\tilde{f}(x)$, which coincides with $f(x)$ on the interval $x \in [0, L]$ and is periodic with period L outside the interval $[0, L]$. In this case, $\tilde{f}(x)$ would not contain the image inside the interval $[0, L]$: for example B, the second “step” would start at the point L , rather than at $L-a$. In this case, the series restores the function exactly inside the interval $[0, L]$ (except for, possibly, the end points $x=0$ and $x=L$). However, the T-series has generated the image $U(L-|x_1-x_2|)$ inside the interval $x \in [0, L]$. Therefore, the series reproduces the function inaccurately. This means, obviously, the simple point: the T-expansion is not the Fourier-expansion for a system with boundaries. In the literature, the T-expansion is called the Fourier-expansion, implying an infinite system, but is applied namely to the systems with boundaries. Below, we will study in detail why the image appears. For clearness, we have started above with simple examples, which can be easily verified. Apparently, this property was not noticed earlier.

Now, we will consider the images more profoundly and will give another way to deduce the T-expansion. We expand $U(|x_1-x_2|)$ in a Fourier series, by considering x_1 and x_2 as arguments (in 1D):

$$U(|x_1-x_2|) = \frac{1}{L_x} \sum_{k_{j_1} k_{j_2}}^{(2\pi)} \nu_2(k_{j_1}, k_{j_2}) e^{ik_{j_1} x_1 + ik_{j_2} x_2}, \quad (20)$$

$$\nu_2(k_{j_1}, k_{j_2}) = \int_0^{L_x} dx_1 \int_0^{L_x} dx_2 U(|x_1-x_2|) e^{-ik_{j_1} x_1 - ik_{j_2} x_2}. \quad (21)$$

In (21), we make change $x_1 = \tilde{x}_1 + x_2$. Then we have

$$\nu_2(k_{j_1}, k_{j_2}) = \int_0^{L_x} dx_2 F(k_{j_1}, x_2) e^{-i(k_{j_1} + k_{j_2})x_2}, \quad (22)$$

$$F(k_{j_1}, x_2) = \int_{-x_2}^{L_x-x_2} d\tilde{x}_1 U(|\tilde{x}_1|) e^{-ik_{j_1} \tilde{x}_1}. \quad (23)$$

For a cyclic system,

$$U(x_1, x_2) = U(x_1 + jL_x, x_2) = U(x_1, x_2 + lL_x) \quad (24)$$

(j and l are integers). Therefore, $U(|-x|) = U(|L_x - x|)$. In view of this, it is easy to show that $F(k_{j_1}, x_2)$ is independent of x_2 : $F(k_{j_1}, x_2) = F(k_{j_1}, 0)$. As a result,

$$\nu_2(k_{j_1}, k_{j_2}) = L_x \nu^c(k_{j_1}) \delta_{k_{j_1}, -k_{j_2}}, \quad (25)$$

$$\nu^c(k_{j_1}) = F(k_{j_1}, 0), \quad (26)$$

$$U(|x_1-x_2|) = \frac{1}{L_x} \sum_{k_j}^{(2\pi)} \nu^c(k_j) e^{ik_j(x_1-x_2)}, \quad (27)$$

where $\delta_{k_{j_1}, -k_{j_2}}$ is the Kronecker symbol. We note that the particle on a ring undergoes the action of another particle from both sides. Therefore,

$$U(|x_1-x_2|) = U_1(|x_1-x_2|) + U_1(L_x - |x_1-x_2|), \quad (28)$$

where U_1 is the potential of such a force. If we open the ring, then relation (28) will contain only the first term. It follows from (28) that $U(|x_1-x_2|) = U(L_x - |x_1-x_2|)$, which agrees with (24). For the potential $U_1(|x_1-x_2|)$, we have

$$F(k_j, 0) = \int_0^{L_x} dx U_1(|x|) e^{-ik_j x}. \quad (29)$$

Let us consider $U_1(L_x - |x_1-x_2|)$. With the help of the change $L_x - |x| = L_x - x = \tilde{x}$ with regard for $e^{ik_j L_x} = 1$, we obtain $F(k_j, 0) = \nu(-k_j)$. Then

$$\begin{aligned} \nu^c(k_j) &= \nu(k_j) + \nu(-k_j) = \\ &= \int_0^{L_x} dx U_1(|x|) (e^{-ik_j x} + e^{ik_j x}) = \int_{-L_x}^{L_x} dx U_1(|x|) e^{-ik_j x}. \end{aligned} \quad (30)$$

Formulas (27), (28), and (30) set the Fourier-expansion of the potential for a cyclic 1D system. If we turn L_x to infinity and neglect the image, then we obtain T-expansion (1), (2) in 1D. This is the proof of the T-expansion.

We note that, at the transition to the T-limit, the potential $U_1(L_x - |x_1-x_2|)$ (image) is usually neglected in (28). But, in our opinion, this is not quite correct, because the topologies of an infinite closed line and an infinite unclosed one are different. The physical potentials $U_1(|x|)$ are large at small $|x|$ and are small at large $|x|$. If we turn $L_x \rightarrow \infty$ in $U_1(L_x - |x_1-x_2|)$, we can also turn x_1 to infinity so that the difference $L_x - |x_1-x_2|$ be small. Then the potential $U_1(L_x - |x_1-x_2|)$ is not small and should not be neglected.

For a cyclic system, the potential $U(|x_1 - x_2|)$ can be expanded in a different way, by considering $|x_1 - x_2|$ or $x_1 - x_2$ as an argument. In this case, it is necessary to take the image into account (see (28)). At the end of this work, we will show that the second way leads again to formulas (27), (28), and (30). Formulas (27), (28), and (30) can be easily generalized to 3D, where the potential has $2^3 - 1 = 7$ images.

Let us return to the system with boundaries. At the expansion, let us consider the arguments x_1 and x_2 to be independent. Then the exact formulas (20) and (21) are valid. The system is uncyclic, and, therefore, the potential has no property (24). Instead of (28), we have

$$U(|x_1 - x_2|) = U_1(|x_1 - x_2|), \quad (31)$$

because no image is present. Let us consider the simple potential (15). With regard for its image for a cyclic system, we obtain

$$\nu^c(k_{j_1}) = \frac{2U_0}{k_{j_1}} \sin k_{j_1} a. \quad (32)$$

For a system with boundaries for $k_{j_1} \neq 0$:

$$F_b(k_{j_1}, x_2) = \begin{cases} F_1(k_{j_1}, x_2), & 0 \leq x_2 < a \\ \nu^c(k_{j_1}), & a < x_2 < L_x - a \\ F_2(k_{j_1}, x_2), & L_x - a < x_2 \leq L_x, \end{cases} \quad (33)$$

$$\begin{aligned} F_1(k_j, x_2) &= \frac{U_0}{k_j} (\sin k_j a + \sin k_j x_2) + \\ &+ \frac{iU_0}{k_j} (\cos k_j a - \cos k_j x_2), \end{aligned} \quad (34)$$

$$\begin{aligned} F_2(k_j, x_2) &= \frac{U_0}{k_j} (\sin k_j a - \sin k_j x_2) + \\ &+ \frac{iU_0}{k_j} (\cos k_j x_2 - \cos k_j a), \end{aligned} \quad (35)$$

$$\nu_2(k_{j_1}, k_{j_2}) = L_x \nu^c(k_{j_1}) \delta_{k_{j_1}, -k_{j_2}} + \tilde{\nu}_2(k_{j_1}, k_{j_2}), \quad (36)$$

$$\tilde{\nu}_2(k_{j_1}, k_{j_2}) = \int_0^a \left[F_1(k_{j_1}, x_2) e^{-i(k_{j_1} + k_{j_2})x_2} + \text{c.c.} \right]. \quad (37)$$

Now, the quantity $\nu_2(k_{j_1}, k_{j_2})$ has a nondiagonal part $\tilde{\nu}_2(k_{j_1}, k_{j_2}) \neq 0$, which is equal to zero for a cyclic system. If we neglect it, we obtain T-expansion (1)-(3). Thus, *the T-expansion is not the exact Fourier-series for an arbitrarily large, but finite system with boundaries; it is only an approximate expansion*, which follows from the exact formulas (20), (36) at the neglect of $\tilde{\nu}_2$. To what extent is this neglect proper? For the real systems, we have $a \ll L_x$, and the nondiagonal addition is small. But sum (20) contains much more nondiagonal terms, than diagonal ones. The role of the nondiagonal contribution can

be easily estimated. Assume that it is insignificant and restore potential (15) with the help of the T-expansion. As a result, we obtain (19), which was mentioned above: the T-expansion adds the image to the initial potential. If we do not reject $\tilde{\nu}_2(k_{j_1}, k_{j_2})$, then series (20), (36) reproduces the initial potential exactly, without any image.

With regard to the limit $L_x \rightarrow \infty$ we can say the following. If we turn continuously $L_x \rightarrow \infty$ in the formulas with a finite L_x , we always have the system with boundaries. In other words, the limiting values for $L_x \rightarrow \infty$ are the values for the arbitrarily large, but finite system. In this case, it is necessary to consider $\tilde{\nu}_2(k_{j_1}, k_{j_2})$; otherwise, the image appears. Thus, such procedure does not allow us to obtain the value for an infinite system without boundaries.

The following mathematical property allowing the better understanding of the role of images is of interest. Let us expand the potential $U(L_x - |x_1 - x_2|)$ of the image in the exact zero-series (6), (7). For any $U(L_x - |x_1 - x_2|)$, we obtain the Fourier-component

$$\nu_{im}(k_j) = (-1)^j \nu_z(k_j), \quad (38)$$

where $\nu_z(k_j)$ is the Fourier-component of the potential $U(|x_1 - x_2|)$, and $k_j = \pi j / L_x$. Then the Fourier-component of the zero-expansion of the potential $U(|x_1 - x_2|) + U(L_x - |x_1 - x_2|)$ reads

$$\tilde{\nu}(k_j) = \begin{cases} 0, & j = 2l + 1, \\ 2\nu_z(k_j), & j = 2l. \end{cases} \quad (39)$$

Substituting it in (6), we obtain the T-expansion: formula (1) with $\nu(k)$ (2). That is, *the T-expansion for a system with boundaries follows from the exact zero-series (6), (7) with regard for images that are really lacking in the system*. In this case, the account for the image changes strongly the Fourier-components of the potential: a half becomes zero, and another half is doubled. Formulas (38), (39) prove also the above assertion that the expansion of a potential in a Fourier series for a cyclic system gives formulas (27), (28), and (30), if $x_1 - x_2$ is taken as the argument of the function.

III. PHYSICAL CONSEQUENCES

The above-presented analysis implies that the T-expansion is not exact for a system with boundaries. But it is usually applied namely to systems with boundaries. The inaccuracy consists in that the T-expansion of the potential $U(|x_1 - x_2|)$ yields the potential $U(|x_1 - x_2|) + U(L_x - |x_1 - x_2|)$ (in 1D). For a finite cyclic system, this feature will give no error in the solution, if the potential in a model is described by the right-hand side of formula (1) (as usual, it is so), since the right-hand side gives the complete cyclic potential $U(|x_1 - x_2|) + U(L_x - |x_1 - x_2|)$. But the situation is different for a system with boundaries. Formula (1) gives $U(|x_1 - x_2|) + U(L_x - |x_1 - x_2|)$, but there is no potential

$U(L_x - |x_1 - x_2|)$ in the system, and the transition from $U(|x_1 - x_2|)$ to $U(|x_1 - x_2|) + U(L_x - |x_1 - x_2|)$ means the transition from a noncyclic complete potential of the system to a cyclic one. This changes the topology of the system. The indicated inaccuracy is small in the meaning that it concerns mainly atoms near the walls of a vessel (the image $U(L_x - |x_1 - x_2|)$ is significant only in the case where one atom is located near one wall, and another atom is positioned near the opposite wall). But this inaccuracy is large in the meaning that it changes the topology of the whole interaction in the system, by making the system closed by the interaction. If the physics of the system is defined by separate atoms, this change should not manifest itself in the bulk properties, since the atom after the collision with a wall quickly “forgets” this wall, by moving inward the vessel and colliding with other atoms. But at very low temperatures (quantum fluids, quantum crystals, and quantum gases) the physics of the system is defined by collective oscillations. These oscillations occur in bulk, but they are modulated by the walls. In this way, the walls can affect the bulk properties. Two mechanisms were proposed for this effect [3].

IV. CONCLUSIONS

The analysis has shown that, for the system with boundaries, the zero-expansion, modulus-expansion, and

a double Fourier series reproduce the interatomic potential $U(|\mathbf{r}_1 - \mathbf{r}_2|)$ exactly. But the usually used T-expansion distorts the potential so that a cyclic potential is obtained instead of the initial noncyclic one; this changes the topology of a problem. From three mentioned exact expansions, the simplest and most suitable for the available methods is that based on the zero-series (6), (7). Our study does not prove that such inaccuracy of the T-expansion will lead necessarily to errors in physical models. The presence or absence of errors should be clarified in the frame of specific physical models. We have presented the reasoning, by which errors should not arise for classical systems, whereas errors are possible, in principle, for quantum systems. Therefore, it is important to properly expand the potential in a series at the simulation of condensed systems. To avoid possible errors, it is better to use the exact Fourier-expansions instead of the standard expansion in the thermodynamic limit.

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